Dr. S. H. Eisman SMUFA - 1312 (L6200) Frankfort Arsenal Philadelphia, Pennsylvania 19137

Dear Dr. Eisman:

This is in reply to your letter of March 15.

No, I have not given much attention to an <u>efficient</u> algorithm for finding the HB-center, since even a scan through every node does not take very long. One of my students did pay some attention to it, but some more urgent problems diverted him. However, I can think of a number of steps that would speed up the search if this became critical. E.g.,

- (a) replace every linear chain by a valued node. A single test will tell if the center is anywhere in that chain.
- (b) choose an arbitrary linear path and label each node on it with the weight of any attached branch. A scan down this path will find the branch that contains the center. Look down it in the same way. Etc.

$$a_0$$
  $a_1$   $a_2$   $a_3$   $a_4$   $a_5$   $a_n$  Let W be the accumulated weight from  $a_n$  to  $a_i$ .

Then the branch rooted at a contains the center if  $W_{j-1} < n/2 \in W_j$  with obvious extensions for equalities.

(c) An extension of b is to choose an arbitrary link and use a similar criterion to ask which of the pair of branches contains the center. The lighter branch need never be weighed again. Then step the links incident on the leading note into the heavier branch, etc. The refinement is hardly worth the trouble (on a large computer) by comparison with the effort of evaluating the radicals, much less preparing the input code. The canonication presumably need be done only once - when the code is interpreted.

However, I do see an application where speed would be important, e.g., in substructure-matching programs where many uncanonical forms may be generated internally. So I thank you for prodding me to think about this.

I saw Gluck's paper. If I had seen it a year ago I would have tried to follow his approach in more detail for the structure generator.

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Dr. S. H. Eisman

We have a plotter/scope display routine now to interpret simple DENDRAL. Of course, it can be dressed up quite a bit, e.g., restore the implicit H's, etc.

Would you like to come out to see this some time? We are thinking of installing a RAND tablet for dynamic input of structures as usual graphs, but this will take some time.

Sincerely yours,

Joshua Lederberg Professor of Genetics

Encl: #120